

Phenanthrene, trimethyl-
30232-26-9 | DTXSID90184328

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 58000 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.58e-01

Confidence level: 6.88e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>9-Anthracenemethanol</div> <div>Measured: 4070</div> <div>Predicted: 5400</div>	<div>Image not found</div> <div>9-Methylanthracene</div> <div>Measured: 64600</div> <div>Predicted: 29700</div>	<div>Image not found</div> <div>Naphthacene</div> <div>Measured: 646000</div> <div>Predicted: 229000</div>
<div>Image not found</div> <div>Benz[a]acridine</div> <div>Measured: 24500</div> <div>Predicted: 154000</div>	<div>Image not found</div> <div>Benz(a)anthracene</div> <div>Measured: 200000</div> <div>Predicted: 227000</div>	